

VI.10 Combustion of Hydrogen in Air under Simulated Accident Conditions (New Project)

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Objectives

- Find from global analysis approximate characteristic time scales determining accident scenarios.
- Initiate detailed modeling of mixing and chemical reaction of hydrogen through direct numerical simulations.

Technical Barriers

This project addresses the following technical barriers from the Codes and Standards section of the Hydrogen Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- A. Limited Government Influence on Model Codes
- B. Competition between ICC and NFPA
- C. Limited State Funds for New Codes
- F. Limited DOE role in the Development of ISO Standards

Approach

- Analyze potential accident scenarios to determine characteristic time scales.
- Review the literature for numerical techniques apt to resolve the chemical scales in direct numerical simulations.
- Determine which of the numerical techniques is compatible with the currently used discretization scheme utilized to solve the equations in the case of mixing.

Accomplishments

- Performed an initial categorization of accident scenarios that is compatible with the Sandia Livermore report of the Unintended Release Workshop, December. 4-5, 2003.
- Obtained preliminary characteristic times for several scenarios.
- Initiated a literature review of novel numerical techniques to resolve the small chemical times in direct numerical simulations.

Future Directions

- The current project began only 2.5 months ago. As we continue with the activities listed above, we will continue with the next stage.
- Continue with evaluations of characteristic times from global analysis.

- Refine the characterization of time scales by considering increasingly specific scenarios.
- Evaluate the potential of novel numerical techniques from the literature to resolve the chemical scales while being compatible with the current discretization scheme for mixing.

Introduction

The future utilization of hydrogen as a fuel leads to safety considerations in the event of unintended leaks. Since leaks can only occur from storage or transportation systems, the system type has direct consequences on the fate of the unintended leak. Currently, there is no systematic analysis and neither is there an estimate of the characteristic times for potential accidents that could lead to defining separation distances through codes and standards. Such analysis must first be of global nature, with necessary refinements introduced by more detailed analysis.

There are four major time scales during unintended hydrogen release: (1) release and possible phase change, (2) mixing time, (3) ignition and (4) propagation. The current work addresses points (1) and the combination of (2), (3) and (4). Accurate knowledge of these time scales will assist DOE to become a participant in determining codes and standards based on quantitative, validated information and through this participation, DOE could assist the states in their decision making process, particularly if the states cannot produce matching quality analysis based on physical principles.

Approach

The approach is based on analysis that relies on firm physical and chemical principles. The strategy is to first obtain order of magnitude characteristic times and categorize scenarios accordingly. In parallel, a more detailed analysis has been initiated that will lead to more accurate characteristic times.

Results

Two types of hydrogen releases are possible: (1) gaseous release and (2) liquid release.

Gaseous hydrogen (GH2) may occur either as an unintended release from a hydrogen tank at high pressure (e.g., 350 bars), hydrogen stored through metal hydrides, hydrogen adsorbed on carbon

nanoparticles or hydrogen stored in clathrate hydrates, as discussed by Mao and Mao (2004).

The gaseous releases can in turn be of two types:

- (i) a burst of the storage system resulting in a short time of release, leading to a cloud of hydrogen, and
- (ii) a jet of hydrogen exiting the tank through a small hole, resulting in a large time for releasing the contents of the tank.

Liquid releases may occur from tanks at 20K. Liquid hydrogen (LH2) releases may result in either: (i) a pool that is heated through contact in such a way that the supplied heat can only gasify the hydrogen through pool boiling without increasing the temperature of the bulk, or (ii) a pool whose bulk is heated up, with ensuing nucleation and hydrogen gasification through flash nucleation. The low latent heat of LH2 suggests that the first process would usually be more important. The last situation will occur if the liquid is heated to about 90% of its critical temperature.

Virtually, all 68 scenarios identified in Schefer et al. (2003) fall under these 4 categories.

Global analysis for gaseous releases led to a range of characteristic times of a few seconds for a tank holding of the order of 1kg of GH2 to 30 minutes for a tank holding 1 GH2 metric ton; in both cases the opening for the release was assumed to be of the order of 1cm² and the pressure in the tank was specified as 340 bar.

Time scales for LH2 pool boiling were obtained by considering the two limiting cases of (1) a confined pool, and (2) an unconfined pool that continuously spreads with time. The first case has been extensively documented in Jurie and Tryggvason (1998) and Dhir (2001), leading to a bubbling evaporation time (in s) that is approximately $2(s/cm) \times H_p(cm)$. In contrast, there is no information on spreading pools, such as shown in Figure 1, where the vapor film that forms between the ground or any heated surface and pool liquid can leak out at the edges, thereby providing an alternate means of vapor escape other than the vapor bubbles

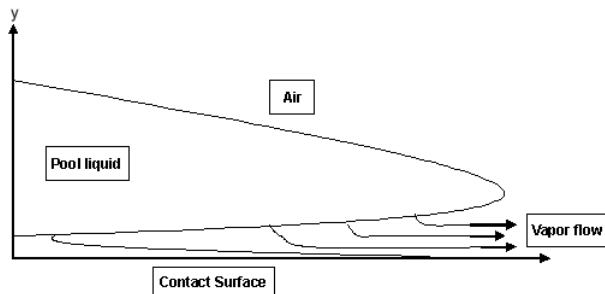


Figure 1. Schematic of Unconfined LH2 Pool Spreading

or jets that escape vertically. A two-dimensional, low Mach number analysis of this film-vapor flow for a cylindrical pool has been conducted and led to an upper characteristic evaporation time (in s) of the edge flow that is approximately $16 \times (A_p H_p^3)^{1/4}$ where lengths are in cm and the proportionality constant has units of $\text{s/cm}^{5/4}$. Thus, the ratio of the characteristic time from bubble escape to that of evaporation through edge effects is approximately $10^{-1} (H_p/A_p)^{1/4} \ll 1$ where the constant has units of $\text{cm}^{1/4}$, meaning that the effect of GH2 release from the edge flow of an expanding pool may be neglected. Therefore, the main effect of pool expansion is that of increasing contact area, which results in a total increase of the GH2 release rate.

Conclusions

A simplified analysis has been conducted to obtain order of magnitude, range and parameter dependencies of typical characteristic times for hydrogen unintended releases. It was found that the numerous release scenarios found in a recent workshop can be actually categorized under four general areas. Global and two-dimensional analyses resulted in estimates of characteristic times that will be further refined with more detailed simulations.

References

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